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TWO ELECTRON CAPTURE

BY

FAST ALPHA PARTICLES IN HELIUM

A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES

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by

EDWARD L. TOMUSIAK

EDMONTON, ALBERTA

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UNIVERSITY OF ALBERTA
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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance, a thesis entitled Two Electron Capture by Fast Alpha Particles in Helium, submitted by Edward L. Tomusiak, in partial fulfillment of the requirements for the degree of Master of Science.

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ABSTRACT

The cross section for the simultaneous capture of two electrons by fast alpha particles in helium is computed in the first Born approximation. Calculations are performed for capture into the ground state ($1S^2$) and the 31S2S state of helium. In both cases the complete interaction Hamiltonian is retained and it is seen that at the lower energies and for ground state capture the matrix elements corresponding to the nucleus-nucleus interaction are comparable in magnitude to those of the Brinkman-Kramers type. With the aid of the Feynman technique are obtained integral expressions, suitable for numerical evaluation, for the matrix elements describing capture into the $1S^2$, 31S2S , 31S2P_x , 11S2P_x , 31S2P_z , and 11S2P_z states. By the subsequent use of Gaussian quadrature integration the matrix elements for $1S^2$ and 31S2S capture are evaluated numerically on an IBM-1620 digital computer.

Aside from the inclusion of the 31S2S state in the capture cross section this work differs from previous calculations in that a two-parameter wave function is used for the ground state of helium. Unfortunately the existing experimental data provides only a few measurements of the total cross section under consideration and at energies where the first Born approximation just begins to be applicable.

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-I- Introduction

The first evidence of charge exchange collisions by high speed particles passing through matter was obtained by Henderson¹, who observed that a beam of alpha particles contains a fraction of singly charged particles which increases with decreasing particle velocity. Since then a wide variety of experimental and theoretical research has been carried out on the general phenomena of charge changing collisions. A good summary of the experimental results until 1952 is presented by Massey and Burhop².

Due to the inherent complexity of electron capture problems (i.e. as pointed out by Bohr³ they are three-body problems in the simplest cases) the theoretical considerations have been rather limited in scope. Although several attempts were made to calculate electron capture cross sections from a classical point of view, it was not until 1928 that Oppenheimer⁴ and especially in 1930 when Brinkman and Kramers⁵ (hereafter referred to as BK) reconsidered the problem quantum mechanically. Following Oppenheimer, BK only considered the (incident particle) - (atomic electron) interaction as the perturbation causing the charge exchange. The cross sections obtained by this method were approximately five to ten times greater than the experimental values of that time. Later, in 1953, Jackson and Schiff⁶ (hereafter referred to as JS) and Bates and Dalgarno⁷ (hereafter referred to as BD) independently, and by different techniques, obtained results in excellent agreement with experiment for the problem of single electron capture by protons in atomic hydrogen. In contrast to the method of BK, BD and JS retained the total interaction Hamiltonian as the perturbation responsible for the charge exchange. G.C. Wick, quoted in a footnote by JS, argued that the (incident particle) - (atomic nucleus) interaction should yield a neg-

ligible contribution to the cross section since in the limit $M/m \gg 1$ the motion of the heavy ions can be treated as classical straight line trajectories. In other words this interaction is a known function of time and can be factored out of the wave equation by an appropriate canonical transformation. However Jackson⁸ advanced a counter argument in which he demonstrated that at energies where $e^2/\hbar v \sim 1$, the transverse momentum impulse given to the atomic electron is comparable to the transverse momentum impulse due to the Coulomb interaction between the two colliding ions. Hence one might expect that near these energies the Fourier components of the separate interactions would interfere destructively thereby lowering the cross section. Jackson also demonstrated that the reason for the JS and BD calculations agreeing so well with experiment was due to the fact that when the nuclear charges are near unity and the complete interaction Hamiltonian is retained then the second Born approximation term nearly vanishes.

One serious objection to the claims of the BD and JS results is that they were compared to the experimental cross sections for protons in molecular hydrogen. Furthermore their cross sections do not seem to have the correct asymptotic behavior in the limit of high incident particle energies. As a result attempts have been recently made by McCarroll⁹, McDowell¹⁰, and others to include the effects of distortion produced on the scattered waves due to the (atomic nucleus) - (electron) potential. These results, although differing from each other slightly in magnitude, all seem to approach the BK cross section at high energies. However it will not be until experiments are performed on atomic hydrogen (if possible) that light will be shed on the merits of any one approximation.

Contrary to the difficulty implied above of performing charge exchange experiments in atomic hydrogen, there is no such problem when considering atomic helium as the target material. Thus in this thesis the Born approx-

imation as applied by JS will be used to compute cross sections for the simultaneous capture of two electrons by fast alpha particles in helium. The implication is not that the experimental work in this regard is complete but that it might be, perhaps, easier to perform than for the case of protons in atomic hydrogen. In fact only a few experimental points have been obtained, by Allison¹¹, and these lie in the region where the first Born approximation just begins to be valid.

The first attempt to compute cross sections for the simultaneous capture of two electrons by alpha particles in helium was by Betts¹² who, after employing the formal method of JS, evaluated the rather cumbersome matrix elements by various approximations. Later Gerasimenko and Rosentsveig¹³ performed a numerical computation for capture into the ground state of helium by approximating, as did Betts, the ground state with a simple one-parameter hydrogenic wave function. The cross sections obtained were an order of magnitude smaller than those of Betts. Here we investigate, again numerically, the effect on the cross section by employing a slightly more complicated wave function for the ground state of helium. The contribution to the cross section from the 31S2S state is also computed and the matrix elements for capture into the triplet and singlet $1S2P$ states are indicated. Finally a few possible refinements on the method are discussed.

-II- Rearrangement Collisions

The formal theory of rearrangement collisions has been treated in an elegant and precise operator formalism by Lippmann¹⁴. Here we will review the summary which Jackson⁸ gave of Lippmann's paper and then apply the results, in the accuracy of the first Born approximation, to rearrangement collisions of alpha particles with helium atoms.

It is customary, in a formal treatment of rearrangement collisions, to speak of an 'initial' and a 'rearranged' system. The Hamiltonian for the total system may be written in either of two ways:

$$H = H_0 + V = H_0' + V' \quad (2-1)$$

where the unprimed quantities refer to the initial system, the primed quantities refer to the rearranged system, H_0 and H_0' are the respective 'unperturbed' Hamiltonians, while V and V' are the respective 'interaction' parts. The unperturbed Hamiltonians have eigenvectors ϕ_α and ϕ_b' such that

$$H_0 \phi_\alpha = E_\alpha \phi_\alpha, \quad H_0' \phi_b' = E_b' \phi_b' \quad (2-2)$$

The operator Green's functions G_0 and G_0' are defined by

$$G_0(\lambda) = \frac{1}{\lambda - H_0}, \quad G_0'(\lambda) = \frac{1}{\lambda - H_0'} \quad (2-3)$$

where $\lambda = E \pm i\epsilon$ for outgoing (+) or incoming (-) waves. The solutions describing incident waves plus scattered waves satisfy the integral equation

$$\bar{\Psi}_\alpha^{(\pm)} = \phi_\alpha + G_0(E_\alpha \pm i\epsilon) V \bar{\Psi}_\alpha^{(\pm)} \quad (2-4)$$

and the corresponding primed equation. If one defines an operator $U(\lambda)$ such that

$$[1 - G_0(\lambda) V] U(\lambda) = 1 \quad (2-5)$$

then equation (2-4) (or its primed equivalent) may be written more compactly as

$$\Psi_a^{(\pm)} = U(E_a \pm i\epsilon) \phi_a \quad (2-6)$$

Lippmann shows, rigorously, that the transition probability for a rearrangement collision is

$$\omega_{ba} = \frac{2\pi}{\hbar} |\langle \phi_b' | V | \Psi_a^{(+)} \rangle|^2 \delta(E_a - E_b) \quad (2-7)$$

and furthermore, that if both H_0 and H_0' are Hermitian

$$\langle \phi_b' | V | \Psi_a^{(+)} \rangle = \langle \Psi_b^{(+)} | V | \phi_a \rangle ; E_b' = E_a \quad (2-8)$$

and also

$$\langle \phi_b' | V | \phi_a \rangle = \langle \phi_b' | V | \phi_a \rangle ; E_b' = E_a \quad (2-9)$$

The first Born approximation consists of replacing $\Psi_a^{(+)}$ by ϕ_a in eqn. (2-7). This corresponds, formally, to a neglect of all terms but the first in the expansion

$$U(\lambda) = 1 + G_0(\lambda)V - G_0(\lambda)V G_0(\lambda)V + \dots \quad (2-10)$$

or its primed equivalent. Thus the differential cross section for a rearrangement collision in which the initial configuration is characterized by ϕ_a and the rearranged system by ϕ_b' is given by the familiar formula

$$d\sigma(\theta, \varphi) = \left(\frac{\mu_f}{2\pi\hbar^2}\right)^2 \frac{v_f}{v_i} |H_{ba}|^2 d\Omega \quad (2-11)$$

where H_{ba} is given by either expression in equation (2-9).

To specialize to the specific problem of two-electron capture by alpha particles in helium we utilize the coordinate system, illustrated in Fig. 1, used by Betts¹² in the same connection. The nuclei are designated by A and B, 1 and 2 are electrons and C_A and C_B are the centers of mass of the initial and final atoms.

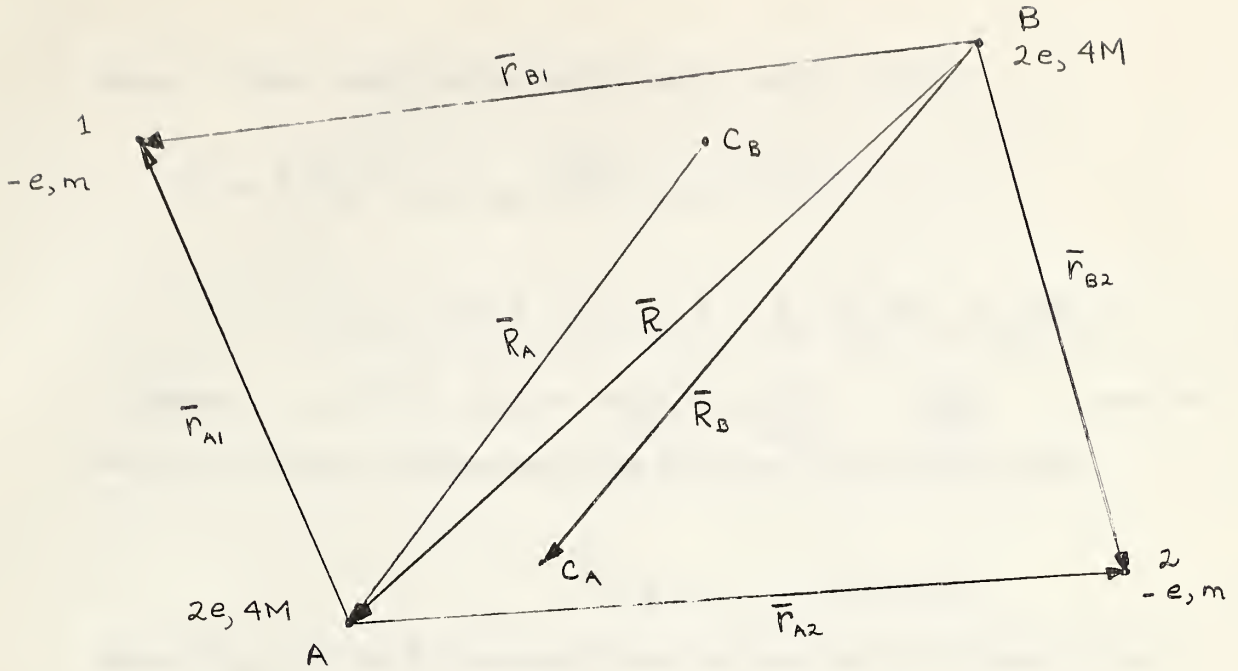


Fig. 1 Coordinate System

If we consider ion B initially incident with relative wave vector \vec{k}_i upon the two-electron atomic arrangement about A and finally a two-electron arrangement about B departing from ion A with relative wave vector \vec{k}_f , we may write

$$\phi_a = \chi_i(\vec{r}_{A1}, \vec{r}_{A2}) e^{i\vec{k}_i \cdot \vec{R}_B}, \quad \phi_b = \chi_f(\vec{r}_{B1}, \vec{r}_{B2}) e^{i\vec{k}_f \cdot \vec{R}_A} \quad (2-12)$$

where $\chi_i(\vec{r}_{A1}, \vec{r}_{A2})$ and $\chi_f(\vec{r}_{B1}, \vec{r}_{B2})$ are the initial and final helium atom wave-functions respectively.

Making the usual assumptions that $|\vec{k}_i| \approx |\vec{k}_f|$ and θ , the scattering angle, is small the momentum transfer may be written as

$$\vec{k}_i \cdot \vec{R}_B - \vec{k}_f \cdot \vec{R}_A = \vec{r}_{B1} \cdot \vec{A} + \vec{r}_{A2} \cdot (\vec{A} + \vec{B}) - \vec{r}_{B2} \cdot \vec{B} \quad (2-13)$$

where

$$a_0^2 A^2 = \left(\frac{v}{v_0}\right)^2 = s^2, \quad a_0^2 B^2 = 4 \left(\frac{v}{v_0}\right)^2 \left(\frac{M \theta}{m}\right)^2 = 4s^2 g^2, \quad \vec{A} \cdot \vec{B} = 0 \quad (2-14)$$

and v_0 is the velocity of an electron in the first Bohr orbit of the hydrogen

atom. Thus, dropping the subscripts b and a, we have

$$H = \int \chi_f^*(\bar{r}_{B1}, \bar{r}_{B2}) V(\bar{R}, \bar{r}_{A1}, \bar{r}_{A2}) \chi_i(\bar{r}_{A1}, \bar{r}_{A2}) \\ \times \exp i[\bar{r}_{B1} \cdot \bar{A} + \bar{r}_{A2} \cdot (\bar{A} + \bar{B}) - \bar{r}_{B2} \cdot \bar{B}] d\bar{r}_{A2} d\bar{r}_{B1} d\bar{r}_{B2} \quad (2-15)$$

Since $V(\bar{R}, \bar{r}_{A1}, \bar{r}_{A2}) = -\frac{2e^2}{r_{A1}} - \frac{2e^2}{r_{A2}} + \frac{4e^2}{R}$, we may write (2-15) more conveniently as the sum of two terms; thus

$$H = H_{(BK)} + H_{(NUC)} \quad (2-16)$$

where $H_{(BK)}$ is the Brinkman-Kramers type matrix element given by

$$H_{(BK)} = -4e^2 \int \chi_f^*(\bar{r}_{B1}, \bar{r}_{B2}) \chi_i(\bar{r}_{A1}, \bar{r}_{A2}) \\ \times \exp i[\bar{r}_{B1} \cdot \bar{A} + \bar{r}_{A2} \cdot (\bar{A} + \bar{B}) - \bar{r}_{B2} \cdot \bar{B}] \frac{1}{r_{A1}} d\bar{r}_{A2} d\bar{r}_{B1} d\bar{r}_{B2} \quad (2-17)$$

and

$$H_{(NUC)} = 4e^2 \int \chi_f^*(\bar{r}_{B1}, \bar{r}_{B2}) \chi_i(\bar{r}_{A1}, \bar{r}_{A2}) \\ \times \exp i[\bar{r}_{B1} \cdot \bar{A} + \bar{r}_{A2} \cdot (\bar{A} + \bar{B}) - \bar{r}_{B2} \cdot \bar{B}] \frac{1}{R} d\bar{r}_{A2} d\bar{r}_{B1} d\bar{r}_{B2} \quad (2-18)$$

-III- Some Simple Hydrogenic Wave Functions for the Ground State and the First Few Excited States of Helium

In this section we shall review some familiar results from the variational method of constructing approximate eigenfunctions for the helium atom. As well we shall present the results of some calculations of 'effective charge' parameters used in simple variational approximations to the $^3\text{1S2S}$, $^3\text{1S2P}$, and $^1\text{1S2P}$ helium wavefunctions.

The well-known variational method consists of first constructing a trial function of an arbitrary number of adjustable parameters, say $\Psi(\vec{r}_1, \alpha_1, \alpha_2, \dots, \alpha_n)$, which satisfies the same boundary or asymptotic conditions as the true eigenfunction. If Ψ is normalized to unity and constructed so that it is orthogonal to the first $j-1$ states, then it can easily be shown that ¹⁵

$$E(\alpha_1, \alpha_2, \dots, \alpha_n) = \langle \Psi | H | \Psi \rangle \geq E_j \quad (3-1)$$

where E_j is the true energy of the j th level and H is the total Hamiltonian of the atom in question. The Hamiltonian for the helium atom may be written as

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - 2e^2\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \quad (3-2)$$

where \vec{r}_1 , \vec{r}_2 are the coordinate vectors of the two electrons and ∇_1^2 and ∇_2^2 are the corresponding Laplacian operators. Since the inequality in eqn. (3-1) is always valid, provided Ψ satisfies the stipulated boundary, normality, and orthogonality conditions, we say that the 'best' choice of the parameters, α_i , is obtained by the n conditions which minimize the energy, $E(\alpha_1, \alpha_2, \dots, \alpha_n)$,

$$\frac{\partial E(\dots \alpha_i \dots)}{\partial \alpha_i} = 0, \quad i = 1, 2, \dots, n. \quad (3-3)$$

The above Hamiltonian is invariant under the group consisting of the two discrete operations of permutation of the two electrons and inversion of the coordinate system and the continuous set of operations of rotation of the coordinate system. As shown for example in Wigner²⁰ the eigenfunctions of the Hamiltonian act as basis functions for the various irreducible representations of the group of H. Hence even if we cannot, as in this case, find the true eigenfunctions we do know what symmetries they possess. Further we are guaranteed by group theoretic considerations that functions of different symmetry in the sense that they belong to different representations of H (or different rows of the same representation in the case of degenerate eigenvalues) are automatically orthogonal. Thus the variational method can be used to find an upper bound to the smallest true eigenvalue corresponding to each different symmetry.

Because of the limitations of time and because as in the protons in hydrogen case only the lowest states are expected to be important, we consider only the subgroup of the discrete operations of inversion and permutation. Under inversion the wave functions may be invariant (even parity) or change sign (odd parity) and likewise under interchange of coordinates of the electrons the wave functions may be invariant (symmetric) or change sign (antisymmetric). In atomic physics the spectroscopic notation for the lowest states of each of these four possible symmetries are

$1S^2$	even symmetric,
31S2S	even antisymmetric,
11S2P	odd symmetric,
31S2P	odd antisymmetric .

The only other state of comparably low energy is the 11S2S state. However as it is of the same symmetry as the unknown $1S^2$ state the variational method cannot guarantee an upper bound to the 11S2S energy level and hence it is not possible to say how good the variational energy levels and wave functions for this state are and so we ignore it in the remainder of this thesis.

A. The ground state ($1S^2$);

The simplest hydrogenic trial function for the ground state of helium, as shown in almost any text on quantum mechanics, is

$$\psi = \left(\frac{z'^3}{\pi a_0^3} \right)^{1/2} e^{-z'/a_0(r_1 + r_2)} \quad (3-4)$$

which when substituted into eqn. (3-1) yields

$$E(z') = \left\{ -2z'^2 + \frac{5}{4}z' + 4z'(z'-2) \right\} R_{He} hc \quad (3-5)$$

The subsequent minimization of $E(z')$ leads to the well known result that

$$E = -5.6953 R_{He} hc \quad \text{for} \quad z' = 27/16 \quad .$$

A slightly more elaborate trial function for the ground state, in the notation of Pauling and Wilson¹⁶, is

$$\psi = N_0(z', z'') [1S_{z'}(1) 1S_{z''}(2) + 1S_{z''}(1) 1S_{z'}(2)] \quad (3-6)$$

where $N_0(z', z'')$ is a normalization factor. Eckart and Hylleraas¹⁷ used this function in a variational treatment and obtained

$$E = -5.7508 R_{He} hc, \quad z' = 2.15, \quad z'' = 1.19$$

as compared to the observed energy of $-5.8074 R_{He} hc$ for the ground state of helium.

B. The 31S2S state;

Here we choose as a trial function

$$\psi_{^31S2S} = N_1(z', z'') [1S_{z'}(1) 2S_{z''}(2) - 2S_{z''}(1) 1S_{z'}(2)] \quad (3-7)$$

where $N_1(z', z'')$, the normalizing factor, is given by

$$N_1(z', z'') = \frac{1}{\sqrt{2}} (1 - A^2)^{-1/2}$$

and

$$A = 2\sqrt{2} \frac{(z' z'')^{3/2} (z' - z'')}{(z' + z'/2)^4} \quad (3-8)$$

Substitution of (3-7) into the energy integral (3-1) yields

$$\frac{E}{R_{He}hc} = \frac{1}{(1-A^2)} \left[(z'^2 + z''^2/4)(1+A^2) - (4z' + z'') + 2AB(4-z'-z'') + P - Q \right] \quad (3-9)$$

where

$$B = \sqrt{2} \frac{(z'z'')^{3/2} (z' - \frac{1}{2}z'')}{(z' + \frac{1}{2}z'')^3} \quad (3-10)$$

$$P = 2A_0 \int 1S_{z'}(1) 2S_{z''}(2) \frac{1}{|\bar{r}_1 - \bar{r}_2|} 1S_{z'}(1) 2S_{z''}(2) d\bar{r}_1 d\bar{r}_2$$

$$= \frac{2(z'z'')}{(2z' + z'')^5} (8z'^4 + 20z'^3z'' + 12z'^2z''^2 + 10z'z''^3 + z''^4) \quad (3-11)$$

and

$$Q = 2A_0 \int 1S_{z'}(1) 2S_{z''}(2) \frac{1}{|\bar{r}_1 - \bar{r}_2|} 1S_{z'}(2) 2S_{z''}(1) d\bar{r}_1 d\bar{r}_2$$

$$= \frac{(z'z'')^3}{16(z' + \frac{z''}{2})^5} \left[80 - \frac{200z''}{(z' + \frac{z''}{2})} + \frac{132z''^2}{(z' + \frac{z''}{2})^2} \right] \quad (3-12)$$

The reader is referred to Appendix 1 for the method of evaluating the integrals P and Q.

Obviously an application of the minimization conditions (3-3) to eqn. (3-9), would be a formidable task. Instead we argue that it is physically reasonable to expect that eqn. (3-9) would be minimized for z' somewhere in a region about $z'=2$ and z'' in a region about $z''=1$. With this in mind a digital computer* was programmed to evaluate eqn. (3-9) for a wide range of points with z' and z'' being incremented (or decremented) in steps of 0.01. Eventually the deepest minimum was found yielding the values

$$E = -4.3333 R_{He}hc, \quad z' = 1.99, \quad z'' = 1.55$$

as compared to the experimental energy of $-4.3504 R_{He}hc$ for the 31S2S state of helium.

* The University of Alberta's IBM-1620, and LGP-30 were used for the variational calculations of this chapter.

C. The $^3\text{IS2P}$ and $^1\text{IS2P}$ states ;

Consistent with the form of the previous trial functions we write here

$$\Psi_{^3\text{IS2P}} = \frac{1}{\sqrt{2}} \left[1s_{z'}(1) 2p_{z''}(2) + 1s_{z'}(2) 2p_{z''}(1) \right] . \quad (3-13)$$

Substitution of eqn. (3-13) into (3-1) yields

$$E_{^3\text{IS2P}} = \left[(z'^2 + z''^2/4) - (4z' + z'') + R + S \right] R_{\text{He}} hc \quad (3-14)$$

where

$$\begin{aligned} R &= 2a_0 \int 1s_{z'}(1) 2p_{z''}(2) \frac{1}{|\vec{r}_1 - \vec{r}_2|} 1s_{z'}(1) 2p_{z''}(2) d\vec{r}_1 d\vec{r}_2 \\ &= 8 \left\{ \frac{z'}{4} - \frac{z'^3 (8z'^3 + 18z'^2 z'' + 15z' z''^2 + 5z''^3)}{(2z' + z'')^5} \right\} \end{aligned} \quad (3-15)$$

and

$$\begin{aligned} S &= 2a_0 \int 1s_{z'}(1) 2p_{z''}(2) \frac{1}{|\vec{r}_1 - \vec{r}_2|} 1s_{z'}(2) 2p_{z'}(1) d\vec{r}_1 d\vec{r}_2 \\ &= \frac{7}{12} \frac{z'^3 z''^5}{(z' + \frac{z''}{2})^7} . \end{aligned} \quad (3-16)$$

Again the reader is referred to Appendix 1 for the method of evaluating the 'coulomb' and 'exchange' integrals R and S respectively.

Finally, numerical minimization of eqn. (3-14) yields the results

$$E_{^3\text{IS2P}} = -4.2612 R_{\text{He}} hc, \quad z' = 1.98, \quad z'' = 1.09,$$

$$E_{^1\text{IS2P}} = -4.2443 R_{\text{He}} hc, \quad z' = 2.00, \quad z'' = 1.00$$

compared to the experimental values of $-4.2663 R_{\text{He}} hc$ and $-4.2476 R_{\text{He}} hc$ respectively.

-IV- Cross Sections for the Simultaneous Capture
of Two Electrons Into the Ground State by
Fast Alpha Particles in Helium

The simple wave function, eqn. (3-4), was first used by Betts¹² and later by Gerasimenko and Rosentsveig¹³ (hereafter referred to as GR) in a computation of cross sections for two-electron capture into the ground state of helium. The cross sections obtained by Betts, based on an approximate evaluation of the BK and nuclear matrix elements, are an order of magnitude higher than those obtained by the semi-numerical procedure of GR.

To serve as a 'starter' for the more elaborate calculations which follow we have also made a numerical computation of ground state capture cross sections using the same wave function as Betts and GR. The pre-numerical manipulations lead to matrix elements expressible as integrals over a unit cube whereas those of GR are over a unit square. However the relative simplicity of our integrands compared to those of GR is sufficient justification for the extra dimension, especially in view of the more complicated wave functions which will be used later on.

The procedure is as follows; inserting expression (3-4) into eqn. (2-17) we have

$$H_{(BK)} = -\frac{4\alpha^6}{\pi^2} \int \exp\left\{-\alpha(r_{A1} + r_{A2} + r_{B1} + r_{B2}) + i(\bar{r}_{B1} \cdot \bar{A} + \bar{r}_{A2} \cdot (\bar{A} + \bar{B}) - \bar{r}_{B2} \cdot \bar{B})\right\} \\ \times \frac{1}{r_{A1}} d\bar{r}_{B1} d\bar{r}_{B2} d\bar{r}_{A2} \quad (4-1)$$

where $\alpha = 27/16q_0$. Introducing the Fourier transforms (viz. Appendix 2)

$$\frac{e^{-\alpha r_{A1}}}{r_{A1}} = \frac{1}{2\pi^2} \int \frac{e^{i\bar{q} \cdot (\bar{r}_{A2} - \bar{r}_{B2} + \bar{r}_{B1})}}{(\alpha^2 + q^2)} d\bar{q}$$

$$e^{-\alpha r_{A2}} = \frac{\alpha}{\pi^2} \int \frac{e^{i\bar{q}_1 \cdot \bar{r}_{A2}}}{(\alpha^2 + q_1^2)^2} d\bar{q}_1 \quad \text{etc. ,}$$

into eqn. (4-1) gives us

$$H_{(BK)} = -\frac{2\alpha^9}{\pi^{10}} \int \exp i \left\{ \bar{r}_{A2} \cdot (\bar{q}_1 + \bar{A} + \bar{B} + \bar{q}) + \bar{r}_{B1} \cdot (\bar{q}_2 + \bar{A} + \bar{q}) + \bar{r}_{B2} \cdot (\bar{q}_3 + \bar{B} + \bar{q}) \right\} \\ \times \frac{d\bar{q} d\bar{q}_1 d\bar{q}_2 d\bar{q}_3 d\bar{r}_{A2} d\bar{r}_{B1} d\bar{r}_{B2}}{(\alpha^2 + q^2)(\alpha^2 + q_1^2)^2(\alpha^2 + q_2^2)^2(\alpha^2 + q_3^2)^2} \quad (4-2)$$

Making use of the Fourier transform of the δ -function,

$$\delta(\bar{r} - \bar{r}_0) = \frac{1}{(2\pi)^3} \int e^{i\bar{k} \cdot (\bar{r} - \bar{r}_0)} d\bar{k} ,$$

eqn. (4-2) readily reduces to

$$H_{(BK)} = -\frac{2^{10}\alpha^9}{\pi} \int \frac{d\bar{q}}{(\alpha^2 + q^2) [\alpha^2 + (\bar{q} + \bar{A} + \bar{B})^2]^2 [\alpha^2 + (\bar{q} + \bar{A})^2]^2 [\alpha^2 + (\bar{q} + \bar{B})^2]^2} \quad (4-3)$$

By the use of a trick introduced by Feynman¹⁸ in another connection we can reduce eqn. (4-3) to a form more appropriate to numerical computation.

Each of the factors in the denominator of (4-3) is expressed in terms of symbols

a, b, c, d and use made of the identity (viz. Appendix 3)

$$\frac{1}{a b^2 c^2 d^2} = 720 \int_0^1 \int_0^1 \int_0^1 \frac{y^2(1-x)(1-y)(1-z)z^4 dx dy dz}{[axyz + byz(1-x) + cz(1-y) + d(1-z)]^7}$$

where we put

$$a = \alpha^2 + q^2 ,$$

$$b = \alpha^2 + (\bar{q} + \bar{A} + \bar{B})^2 ,$$

$$c = \alpha^2 + (\bar{q} + \bar{A})^2 ,$$

and

$$d = \alpha^2 + (\bar{q} + \bar{B})^2 .$$

Simple algebraic manipulations lead us to the result

$$H_{(BK)} = -\frac{2^{10}\alpha^9}{\pi} (720) \int_0^1 \int_0^1 \int_0^1 y^2(1-x)(1-y)(1-z)z^4 dx dy dz \int \frac{d\bar{q}}{\{(\bar{q} + \bar{A})^2 + q^2\}^7} \quad (4-4)$$

where

$$\begin{aligned}\bar{A} &= \bar{A}C_1 + \bar{B}C_2 \\ \eta^2 &= \alpha^2 + A^2C_1(1-C_1) + B^2C_2(1-C_2) \\ C_1 &= z(1-xy)\end{aligned}$$

and

$$C_2 = 1 - z + yz - xyz$$

Finally when use is made of the well-known result

$$I_\ell = \int \frac{d^3k}{(k^2 + \beta^2)^\ell} = \frac{\pi^2 (2\ell-5)!!}{(\ell-1)! 2^{\ell-2} \beta^{2\ell-3}} \quad (4-5)$$

eqn. (4-4) reduces to

$$H_{(BK)} = -30,240 \alpha^9 \pi \int_0^1 \int_0^1 \int_0^1 \frac{y^2(1-x)(1-y)(1-z)z^4 dx dy dz}{[A^2C_1(1-C_1) + B^2C_2(1-C_2) + \alpha^2]^{1/2}} \quad (4-6)$$

It is noted that when JS applied the above methods to the protons in hydrogen problem the integrals defining the nuclear and BK matrix elements could be evaluated exactly. In the present case however we have two equivalent integrals, (4-3) and (4-6), neither of which can be analytically integrated. Inspection of (4-3) shows that the integrand is very sharply peaked near $q=0$, $\bar{q} = -(\bar{A} + \bar{B})$, $\bar{q} = -\bar{A}$, and $\bar{q} = -\bar{B}$. This was the basis for the approximate evaluation of the integral by Betts. However it is very difficult to find a numerical procedure which will take advantage of the fact that the chief contribution to the integral comes from the above points, especially when each evaluation of the integral will be for a different value of A or B or both. Hence the superiority of (4-6) to (4-3) in a numerical computation is clear since in (4-6) the peaking is not so evident and the range of integration is drastically reduced.

The nuclear matrix element is attacked in a similar manner to that outlined above. Substituting (3-4) into eqn. (2-18) and again introducing the appropriate Fourier transforms for $1/R$, etc. (see Appendix 2), leads us to

$$H_{(NUC)} = \frac{2^{10} \alpha^{10}}{\pi^3} \int \frac{d\vec{q} d\vec{p}}{p^2 (\alpha^2 + q^2) [\alpha^2 + (\vec{q} - \vec{p} - \vec{B})^2]^2 [\alpha^2 + (\vec{q} - \vec{A})^2]^2 [\alpha^2 + (\vec{q} - \vec{p} - \vec{A} - \vec{B})^2]^2} \quad (4-7)$$

Eqs. (4-3) and (4-7) are the same as Betts' (4-3) and (4-4). The reduction of eqn. (4-7) to a form suitable for numerical evaluation is outlined as follows.

Considering first the integration over p-space only we have

$$I = \int \frac{d\vec{p}}{p^2 [\alpha^2 + (\vec{p} - \vec{C})^2]^2 [\alpha^2 + (\vec{p} - \vec{D})^2]^2}$$

where $\vec{C} = \vec{q} - \vec{B}$ and $\vec{D} = \vec{q} - \vec{A} - \vec{B}$. Introducing the Feynman auxiliary integral

$$\frac{1}{(ab)^2} = \int_0^1 \frac{6x(1-x) dx}{[ax + b(1-x)]^4}$$

one obtains by choosing

$$a = \alpha^2 + p^2 + C^2 - 2\vec{p} \cdot \vec{C}$$

and

$$b = \alpha^2 + p^2 + D^2 - 2\vec{p} \cdot \vec{D}$$

that

$$I = \int_0^1 6x(1-x) dx \int \frac{d\vec{p}}{p^2 [p^2 + \Delta - 2\vec{p} \cdot \vec{\xi}]^4}$$

where

$$\Delta = C^2 x + D^2 (1-x)$$

and

$$\vec{\xi} = x\vec{C} + (1-x)\vec{D} \quad .$$

Since

$$\int \frac{d\vec{p}}{p^2 [p^2 + \Delta - 2\vec{p} \cdot \vec{\xi}]^2} = \frac{\pi^2}{(\Delta - \xi^2)^{1/2} \Delta}$$

we have that

$$I = \int_0^1 x(1-x) \frac{\partial^2}{\partial \Delta^2} \left\{ \frac{\pi^2}{(\Delta - \xi^2)^{1/2} \Delta} \right\} dx$$

$$= \pi^2 \int_0^1 x(1-x) \left\{ \frac{3/4}{(\Delta - \xi^2)^{5/2} \Delta} + \frac{1}{(\Delta - \xi^2)^{3/2} \Delta^2} + \frac{2}{(\Delta - \xi^2)^{1/2} \Delta^3} \right\} dx \quad .$$

Fortunately the term $(\Delta - S^2)$ does not depend on the variable \bar{q} and hence, since the Δ 's are raised only to interger powers, the Feynman technique can be used again to treat the remaining \bar{q} -space part of eqn. (4-7). We eventually get

$$H_{(NUC)} = 480 \pi \alpha^{10} \int_0^1 \int_0^1 \int_0^1 \frac{xy^2(1-x)(1-y)(1-z)}{F^{1/2} \beta^7} \left\{ \frac{3}{F^2} + \frac{14C_2}{F\beta^2} + \frac{63C_2^2}{\beta^4} \right\} dx dy dz \quad (4-8)$$

where

$$F = \alpha^2 + x(1-x)A^2$$

$$\beta^2 = A^2 C_1(1-C_1) + B^2 C_2(1-C_2) + \alpha^2$$

$$C_1 = 1 - \gamma + \gamma z - xyz$$

and

$$C_2 = \gamma z$$

The quantities c_1 and c_2 appearing in eqns. (4-6) and (4-8) are defined differently in each case. Due to the enormous number of definable terms which occur in this type of work the policy adopted throughout this thesis has been to assign the same symbols to terms which appear in the same algebraic manner throughout the manipulations. Thus following each final statement of a matrix element there will usually appear a list of symbol definitions.

For an indication as to which numerical procedure would do the most justice to (4-6) and hence, it is presumed, to (4-8) use was made of the fact that (4-3) can be integrated exactly for the case of zero scattering angle ($g=0=B$). In fact

$$H_{(BK)}(0) = -2^7 \pi \alpha^4 \frac{(336\alpha^4 + 24\alpha^2 S^2 + S^4)}{(4\alpha^2 + S^2)^5}$$

It was found that the use of eight points along each axis in a Legendre-Gauss quadrature technique¹⁹ gave at least four figure accuracy in the range $S^2 = \alpha^2$ to $S^2 = 8\alpha^2$. With a non-zero g and a fixed value of S^2 the results of the numerical integrations converged to at least four figure agreement when

the number of abscissae per axis was greater than seven. Thus, although the nature of the error arising from the application of the above method to the nuclear integral of eqn. (4-8) and to the more complicated matrix elements which follow is not quite so clear, this is the numerical technique used from here on throughout the thesis i.e. an 8-point Legendre-Gauss quadrature formula. All matrix elements were evaluated on the University of Alberta's IBM - 1620 at an average time of 3/4 of an hour for each evaluation of a BK element and 1 and 1/4 hours for each evaluation of a nuclear matrix element. Furthermore each matrix element was evaluated at several different values of S^2 and, at each of these values of S^2 , over a suitably wide range of values of g .

The total capture cross section into a given state is obtained from eqn. (2-11) by making the approximations

$$\mu_f \approx 2M, \quad d\Omega = \pi \left(\frac{m}{M}\right)^2 d(g^2), \quad v_i = v_f$$

and thus

$$\frac{\sigma}{\pi a_0^2} = \frac{1}{\pi^2} \int_0^\infty |H_{(BK)} + H_{(Nuc)}|^2 d(g^2) \quad (4-9)$$

The methods employed when using the improved wave function (3-6) to evaluate the ground state capture cross section are similar to those above.

We obtain

$$H_{(BK)} = -30,240 \pi N_0^2 (ab)^4 \int_0^1 \int_0^1 \int_0^1 dx dy dz \, y^2(1-x)(1-y)(1-z) z^4 \\ \times \left\{ \frac{b}{(\beta_{AB}^2 + \xi_{ab})^{1/2}} + \frac{a}{(\beta_{AB}^2 + \xi_{ba})^{1/2}} + \frac{b}{(\beta_{BA}^2 + \xi_{ab})^{1/2}} + \frac{a}{(\beta_{BA}^2 + \xi_{ba})^{1/2}} \right\} \quad (4-10)$$

where

$$\beta_{AB}^2 = A^2 C_1(1-C_1) + B^2 C_2(1-C_2) \quad ,$$

$$\beta_{BA}^2 = B^2 C_1(1-C_1) + A^2 C_2(1-C_2) \quad ,$$

$$\begin{aligned}
 \xi_{ab} &= a^2 yz + b^2 (1-yz) & , \\
 \xi_{ba} &= b^2 yz + a^2 (1-yz) & , \\
 C_1 &= 1 - z + yz - xyz & , \\
 C_2 &= 1 - yz & , \\
 a &= 2.15 \quad , \quad b = 1.19
 \end{aligned}$$

and

$$N_0 = \frac{1}{\sqrt{2}} \left[\frac{(a+b)^6}{(a+b)^6 + 64(ab)^3} \right]^{1/2} .$$

With a, b, and N_0 defined as above the nuclear term yields

$$\begin{aligned}
 H_{(Nuc)} &= 480 N_0^2 \pi (ab)^5 \int_0^1 \int_0^1 \int_0^1 dx dy dz \quad xy^2(1-x)(1-y)(1-z) \\
 &\times \sum_{i=1}^4 \frac{1}{F_i^{1/2} (\beta^2 + \xi_i)^{7/2}} \left\{ \frac{3}{F_i^2} + \frac{14 C_2}{F_i (\beta^2 + \xi_i)} + \frac{63 C_2^2}{(\beta^2 + \xi_i)^2} \right\} \quad (4-11)
 \end{aligned}$$

where

$$\begin{aligned}
 F_1 &= b^2 + x(1-x)A^2 & , \\
 F_2 &= a^2 x + b^2(1-x) + x(1-x)A^2 & , \\
 F_3 &= b^2 x + a^2(1-x) + x(1-x)A^2 & , \\
 F_4 &= a^2 + x(1-x)A^2 & , \\
 C_1 &= 1 - y + yz - xyz \quad , \quad C_2 = yz & , \\
 \xi_1 &= b^2 C_2 + a^2 (1 - C_2) & , \\
 \xi_2 &= b^2 C_1 + a^2 (1 - C_1) & , \\
 \xi_3 &= a^2 C_1 + b^2 (1 - C_1) & ,
 \end{aligned}$$

and

$$\xi_4 = a^2 C_2 + b^2 (1 - C_2) .$$

Tables 1 and 2 depict the calculated values of $H_{(BK)}$ and $H_{(Nuc)}$ from formulae (4-10) and (4-11) respectively. A comparison of these results with those using the simple wave function obtained above and those of GR is illustrated in Fig. 2.

Table 1

The following is a listing of the values of $H_{(B\kappa)}$ (times minus one) as computed from the two-parameter wave function for the ground state of helium using eqn. (4-10).

g	$S^2 = \alpha^2$	$S^2 = 2\alpha^2$	$S^2 = 3\alpha^2$	$S^2 = 4\alpha^2$	$S^2 = 6\alpha^2$	$S^2 = 8\alpha^2$
0.0	16.1357	6.7832	3.3494	1.8479	0.7074	0.3325
0.1	15.4321	6.2672	3.0049	1.6141	0.5881	0.2637
0.2	13.5475	5.0015	2.2211	1.1177	0.3647	0.1488
0.3	11.0200	3.5472	1.4242	0.6621	0.1916	0.0715
0.4	8.4136	2.3105	0.8337	0.3584	0.0931	0.0323
0.5	6.1127	1.4234	0.4636	0.1857	0.0440	0.0144
0.6	4.2813	0.8491	0.2522	0.0951	0.0209	0.0065
0.7	2.9241	0.4994	0.1369	0.0491	0.0102	0.0031
0.8	1.9662	0.2935	0.0753	0.0259	0.0051	
0.9	1.3118	0.1740	0.0423	0.0141		
1.0	0.8739	0.1048	0.0244	0.0080	0.0015	0.0004
1.1	0.5840	0.0643		0.0046		
1.2	0.3929	0.0403		0.0028		
1.3	0.2669			0.0017		
1.4	0.1833			0.0011		
1.5	0.1274	0.0113	0.0024	0.0007	0.0001	0.0000
1.6	0.0897			0.0005		
1.7	0.0640			0.0003		
1.8						
1.9						
2.0	0.0251					
2.5		0.0005				
3.0	0.0022					

Table 2

The following is a listing of the values of $H_{(Nuc)}$ as computed from the two parameter wave function for the ground state of helium using eqn. (4-11).

g	$S^2 = \alpha^2$	$S^2 = 2\alpha^2$	$S^2 = 3\alpha^2$	$S^2 = 4\alpha^2$	$S^2 = 6\alpha^2$	$S^2 = 8\alpha^2$
0.0	11.0890	4.1739	1.8671	0.9421	0.3074	0.1256
0.1	10.7458	3.9542	1.7373	0.8632	0.2742	0.1094
0.2	9.8081	3.3932	1.4236	0.6816	0.2042	0.0777
0.3	8.5012	2.6993	1.0689	0.4907	0.1386	0.0507
0.4	7.0775	2.0476	0.7674	0.3399	0.0920	0.0328
0.5	5.7310	1.5200	0.5453	0.2355	0.0621	0.0219
0.6	4.5675	1.1266	0.3921	0.1669	0.0435	0.0153
0.7	3.6193	0.8450	0.2889	0.1222	0.0317	
0.8	2.8739	0.6460	0.2189	0.0923	0.0240	
0.9	2.2994	0.5048	0.1705	0.0719		
1.0	1.8601	0.4030	0.1361	0.0574	0.0149	0.0052
1.1	1.5251	0.3282		0.0468		
1.2	1.2653	0.2719		0.0388		
1.3	1.0640			0.0326		
1.4	0.9055			0.0277		
1.5	0.7791	0.1677	0.0566	0.0238	0.0061	0.0021
1.6				0.0206		
1.7				0.0179		
1.8				0.0157		
1.9						
2.0	0.4161					
2.5		0.0526				
3.0	0.1665					

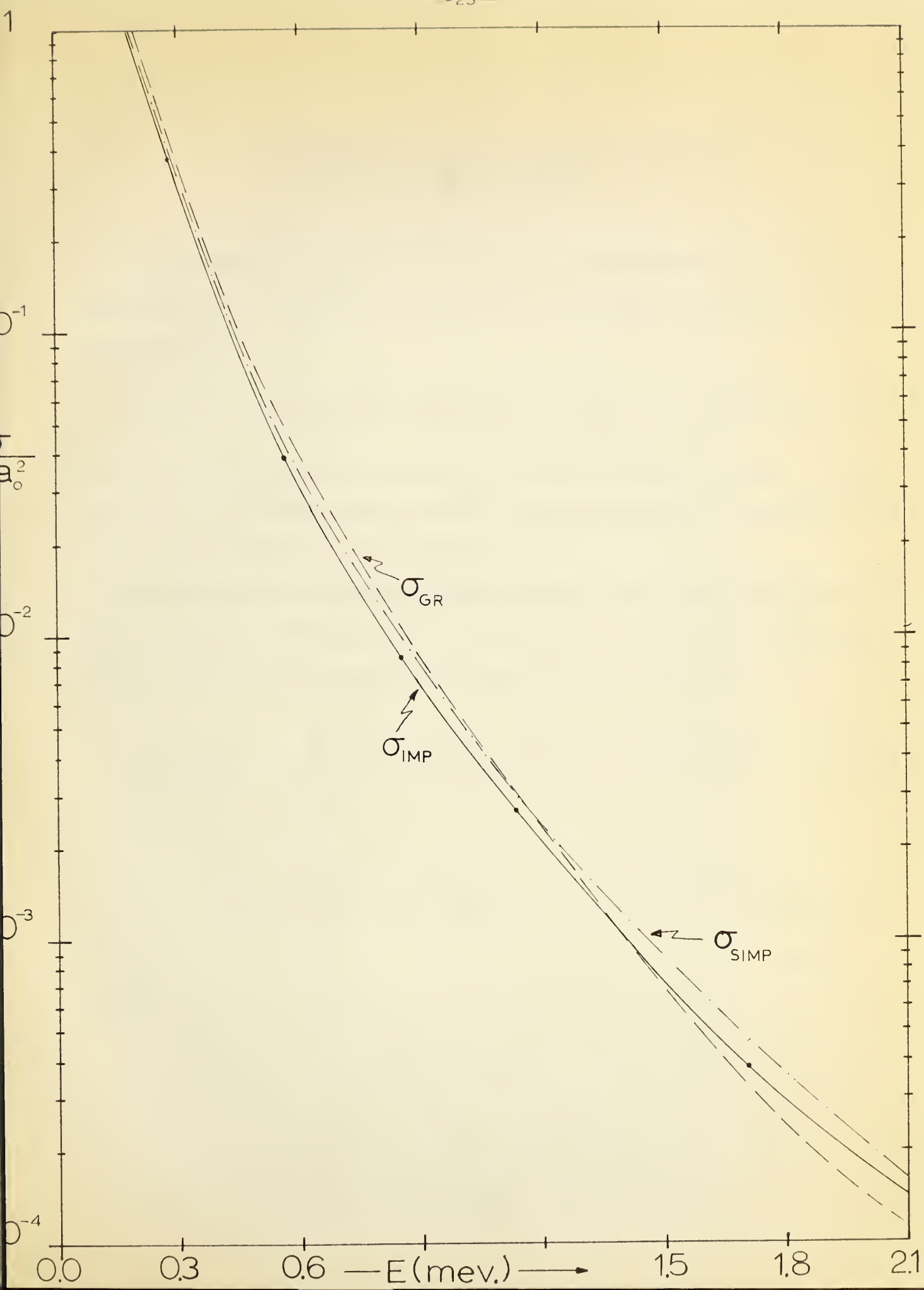
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Figure 2

Cross sections for the simultaneous capture into the ground state of two electrons by fast alpha particles in helium: _____ represents the improved calculations, σ_{IMP} ; ____ . ____ . ____ . represents our cross section, σ_{SIMP} , arising from the simple wave function and _____ depicts the results of GR, σ_{GR} .



-V- Cross Sections for the Simultaneous Capture of
Two Electrons into Excited States by Fast Alpha
Particles in Helium

The differential cross section for a capture process whereby one electron is taken into an 'n=1 state' and the other into an 'n=2 state' is indicated by the proportionality

$$\sigma_{1,2} \propto |H_{11S2S}|^2 + |H_{31S2S}|^2 + \sum_{j=x,y,z} \left\{ |H_{11S2P_j}|^2 + |H_{31S2P_j}|^2 \right\}.$$

In this section we present calculations of the cross section, σ_{31S2S} . Matrix elements for the singlet and triplet 1S2P capture processes are derived and left in a form amenable to numerical evaluation.

Substitution of the wave function (3-7) into eqns. (2-17) and (2-18) plus manipulations similar to those outlined in the previous section yields the following BK and nuclear matrix elements for capture into the 31S2S state:

$$\begin{aligned} \frac{H(BK)}{434,240} &= \sum_{i=1}^2 d_i \left[\int_0^1 \int_0^1 \int_0^1 \frac{T}{(\beta + n_i)^{1/2}} \left\{ \frac{11\alpha_i^2 z(1-\gamma)}{(\beta + n_i)} - 2 \right\} dx dy dz \right] \\ &+ \sum_{i=3}^4 d_i \left[\int_0^1 \int_0^1 \int_0^1 \frac{T}{(\beta + n_i)^{1/2}} \left\{ 2 - \frac{11\alpha_i^2 \gamma z(1-\gamma)}{(\beta + n_i)} \right\} dx dy dz \right] \end{aligned} \quad (5-1)$$

where

$$\begin{aligned} d_1 &= d_3 = b = 1.19, \\ d_2 &= d_4 = a = 2.15, \\ \alpha_1 &= 1.99, \quad \alpha_2 = 0.78, \\ T &= \gamma^2(1-x)(1-\gamma)(1-z)z^4, \\ \beta &= A^2 C_1(1-C_1) + B^2 C_2(1-C_2), \end{aligned}$$

$$C_1 = 1 - z + yz - xyz, \quad C_2 = 1 - yz, \\ n(p; q; r; s) = pxyz + qyz(1-x) + rz(1-y) + s(1-z), \\ n_1 = n(\alpha^2; \alpha_1^2; \alpha_2^2; b^2), \quad n_2 = n(b^2; \alpha_1^2; \alpha_2^2; a^2), \\ n_3 = n(\alpha^2; \alpha_2^2; \alpha_1^2; b^2), \quad n_4 = n(b^2; \alpha_2^2; \alpha_1^2; a^2)$$

and

$$\frac{H_{(NUC)}}{17,635} = \sum_{i=1}^2 \left[\int_0^1 \int_0^1 \int_0^1 \frac{1}{F_i^{1/2} \beta_i^7} \left\{ T_A \left(\frac{6}{F_i^2} + \frac{28C_2}{F_i \beta_i^2} + \frac{126C_2^2}{\beta_i^6} \right) \right. \right. \\ \left. \left. - \alpha_2^2 T_B \left(\frac{15}{F_i^3} + \frac{63C_2}{F_i^2 \beta_i^2} + \frac{189C_2^2}{F_i \beta_i^4} + \frac{693C_2^3}{\beta_i^6} \right) dx dy dz \right] \right. \\ \left. + \sum_{i=3}^4 \left[\int_0^1 \int_0^1 \int_0^1 \frac{1}{F_i^{1/2} \beta_i^7} \left\{ \alpha_2^2 T_C \left(\frac{21}{F_i^2 \beta_i^2} + \frac{126C_2}{F_i \beta_i^4} + \frac{693C_2^2}{\beta_i^6} \right) \right. \right. \right. \\ \left. \left. - T_A \left(\frac{6}{F_i^2} + \frac{28C_2}{F_i \beta_i^2} + \frac{126C_2^2}{\beta_i^4} \right) \right\} dx dy dz \right] \quad (5-2)$$

where

$$T_A = xyz(1-x)(1-y)(1-z), \quad T_B = x T_A, \quad T_C = (1-y) T_A,$$

$$\left. \begin{aligned} F(t; u) &= tx + u(1-x) + x(1-x)A^2 \\ F_1 &= F(\alpha_2^2; b^2), \quad F_2 = F(\alpha_2^2; a^2) \\ F_3 &= F(\alpha_1^2; b^2), \quad F_4 = F(\alpha_1^2; a^2) \end{aligned} \right\} \quad (5-3)$$

$$\beta_m = [A^2 C_1 (1-C_1) + B^2 C_2 (1-C_2) + g_m]^{1/2}, \quad (5-4)$$

$$C_1 = 1 - y + yz - xyz, \quad C_2 = yz, \quad (5-5)$$

$$\left. \begin{aligned} f(p; q; r; s) &= pxyz + qyz(1-x) + ry(1-z) + s(1-y), \\ f_1 &= f(\alpha_2^2; b^2; a^2; \alpha_1^2), \quad f_2 = f(\alpha_2^2; a^2; b^2; \alpha_1^2), \\ f_3 &= f(\alpha_1^2; b^2; a^2; \alpha_2^2), \quad f_4 = f(\alpha_1^2; a^2; b^2; \alpha_2^2), \end{aligned} \right\} \quad (5-6)$$

and as above

$$a = 2.15, \quad b = 1.19, \quad \alpha_1 = 1.99, \quad \alpha_2 = 0.78.$$

Tables 3 and 4 list the values of $H_{(BK)}$ and $H_{(NOC)}$ calculated from the above equations while Fig. 3 illustrates a comparison between the cross section for $1S^2$ (as given by Fig. 2) and 31S2S capture by plotting the ratio $100 \sigma_{^31S2S} / \sigma_{1S^2}$ against the energy of the incident ion. Finally Fig. 4 illustrates the cross section $\sigma = \sigma_{1S^2} + \sigma_{^31S2S}$ along with the experimental points of Allison.

Since the $1S2P$ states are not represented by spherically symmetric wave functions we must specify directions for the vectors \bar{A} and \bar{B} . We choose them such that \bar{A} and \bar{B} define the x and z axes respectively of the final state wave function. Such being the choice we have thus eliminated the contribution to the cross section $\sigma_{1,2}$ from all the $1S2P_y$ states. This is clear upon realization that the perturbations causing the capture are rotationally invariant and that with \bar{A} and \bar{B} chosen as they are the introduction of the $1S2P_y$ wave functions into either of eqns. (2-17) or (2-18) is tantamount to averaging a function of odd parity over all space. Of course this result will readily appear upon a detailed examination of the matrix elements for these states.

To begin with we shall deal with the BK terms for the triplet and singlet $1S2P_z$ and $1S2P_x$ states. Although the procedure of applying Fourier transforms, etc. is identical to that outlined in the previous section, several different types of integrals occur which are worthy of mention. These integrals occur in the same

Table 3

The following is a listing of the values of $H_{(Bk)}$ for capture into the triplet 1S2S state as computed from eqn. (5-1).

g	$S^2 = \alpha^2$	$S^2 = 2\alpha^2$	$S^2 = 3\alpha^2$	$S^2 = 4\alpha^2$	$S^2 = 6\alpha^2$
0.0	-3.2504	-1.3879	-0.6344	-0.3127	-0.0838
0.1	-2.8000	-1.0621	-0.4243	-0.1780	-0.0277
0.2	-1.8076	-0.4996	-0.1355	-0.0298	0.0101
0.3	-0.8937	-0.1622	-0.0212	0.0060	0.0081
0.4	-0.3436	-0.0447	-0.0009	0.0048	0.0031
0.5	-0.1022	-0.0166	-0.0008	0.0015	0.0010
0.6	-0.0241	-0.0103	-0.0014	0.0002	0.0002
0.7	-0.0073	-0.0072	-0.0013	-0.0002	-0.0001
0.8	-0.0057	-0.0046	-0.0009	-0.0003	
0.9	-0.0050	-0.0027	-0.0007	-0.0003	
1.0	-0.0030	-0.0016	-0.0005	-0.0002	
1.1	-0.0007	-0.0010	-0.0005		
1.2	0.0011	-0.0008	-0.0004		
1.3	0.0021	-0.0007			
1.4	0.0025	-0.0006			
1.5	0.0023	-0.0005			
1.6	0.0019				
1.7	0.0014				
1.8	0.0009				
1.9	0.0004				
2.0	0.0001				

Table 4

The following is a listing of the values of $H_{(Nuc)}$ for capture into the triplet 1S2S state as computed from eqn. (5-2).

g	$S^2 = \alpha^2$	$S^2 = 2\alpha^2$	$S^2 = 3\alpha^2$	$S^2 = 4\alpha^2$
0.0	-0.1462	-0.1075	-0.0678	-0.0404
0.1	-0.1353	-0.0934	-0.0558	-0.0317
0.2	-0.1103	-0.0661	-0.0354	-0.0182
0.3	-0.0843	-0.0440	-0.0212	
0.4	-0.0643	-0.0299	-0.0129	
0.5	-0.0504	-0.0207	-0.0079	
0.6	-0.0406	-0.0144	-0.0047	
0.7	-0.0330	-0.0098	-0.0027	
0.8	-0.0267	-0.0065	-0.0014	
0.9	-0.0213	-0.0043		
1.0	-0.0167	-0.0027		
1.1	-0.0129			
1.2	-0.0098			
1.3	-0.0074			
1.4	-0.0054			
1.5	-0.0039			

Figure 3

The ratio $100 \sigma_{31s2s} / \sigma_{1s^2}$ is plotted against the energy of the incident ion.

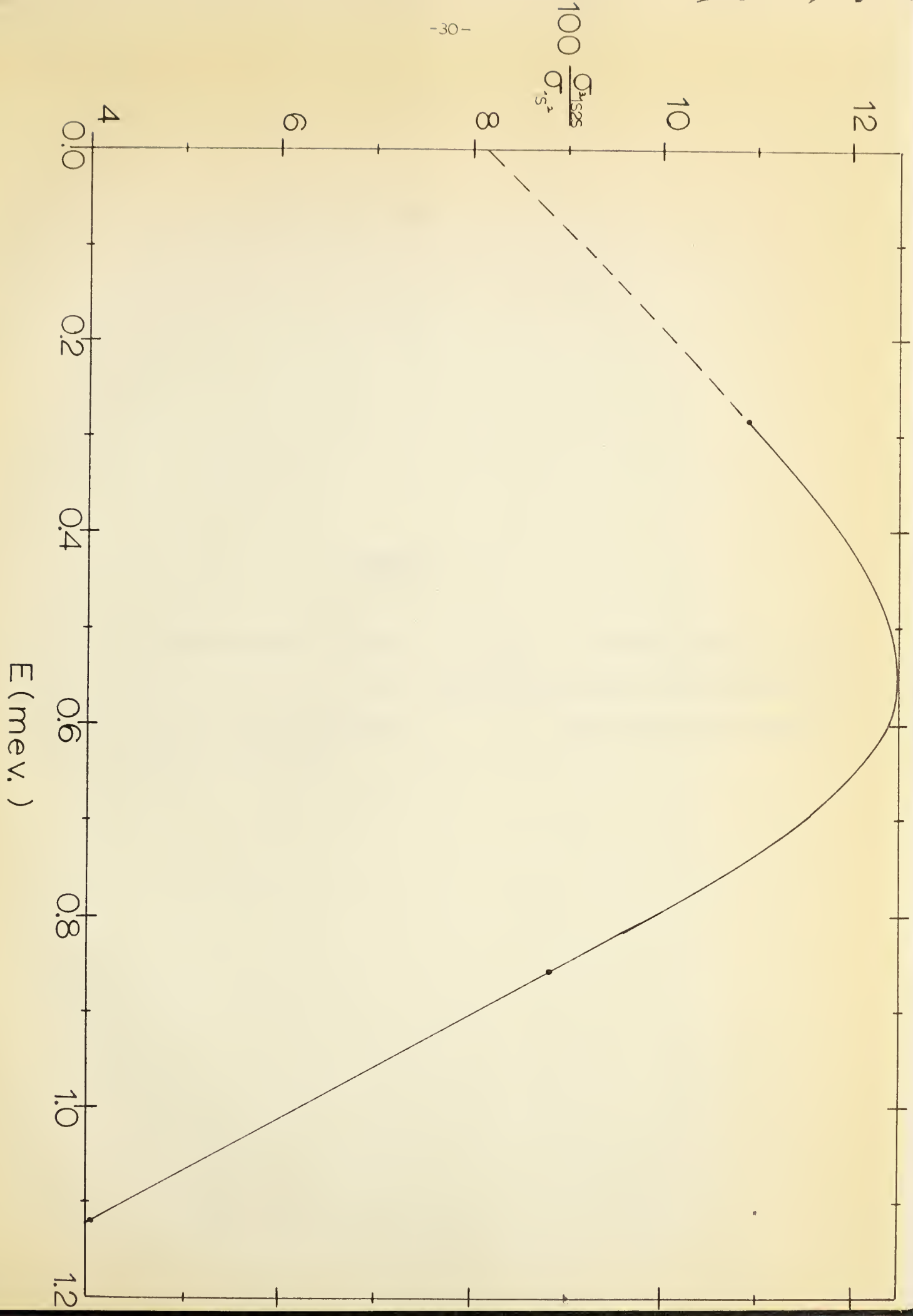
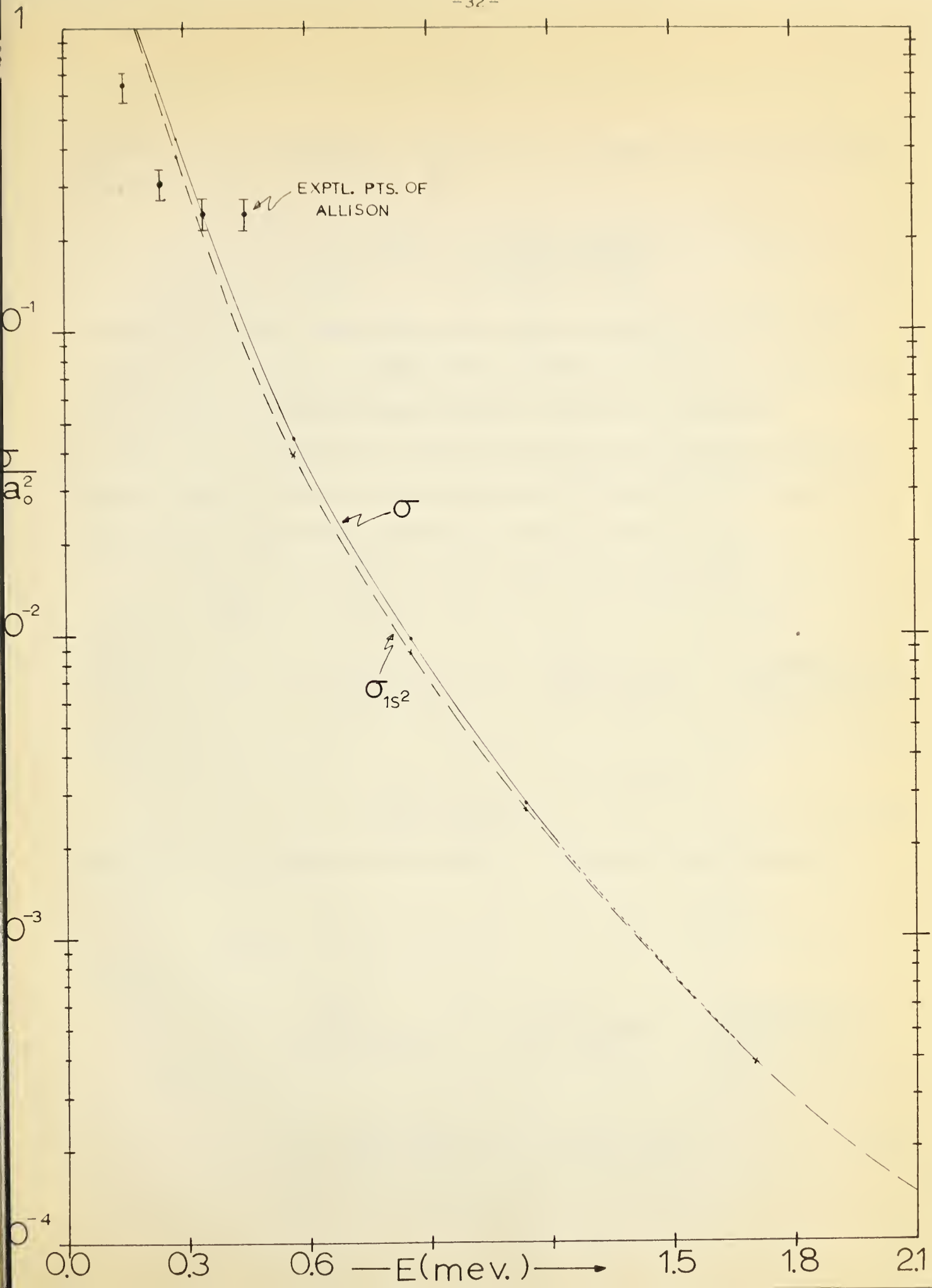


Figure 4

The cross section $\sigma = \sigma_{132} + \sigma_{3132s}$ is illustrated by the solid curve _____. For comparison the cross section σ_{132} (or σ_{imp}) is shown by the dashed curve _____. The experimental points of Allison are indicated.



fashion as did the integral I_ℓ of eqn. (4-5). The general form of the integral which occurs is

$$J_\ell^{(x,y,z)} = \int \frac{q_{x,y,z} d\vec{q}}{[(\vec{q} + \vec{\Lambda})^2 + \gamma^2]^\ell} \quad (5-7)$$

where $\vec{\Lambda}$ is a linear combination of the vectors \vec{A} and \vec{B} (i.e. $\vec{\Lambda} = \vec{A}c_1 + \vec{B}c_2$) and q_x , q_y , and q_z are defined by the directions of \vec{A} , $\vec{B} \times \vec{A}$, and \vec{B} respectively. A method of evaluating these integrals is outlined in Appendix 4.

In the final results which are shown below the upper sign (when two signs appear) applies to capture in the appropriate triplet state and the lower sign applies to the singlet state. Thus for the $1S2P_z$ states we have

$$\begin{aligned} \frac{H_{BK}}{N} = & B \int_0^1 \int_0^1 \int_0^1 \gamma^2 (1-x)(1-y)(1-z)^2 z^4 \\ & \times \left\{ \pm \frac{bc_1}{(\beta_{BA} + \xi_{ab})^{1/2}} \pm \frac{ac_1}{(\beta_{BA} + \xi_{ba})^{1/2}} - \frac{b(1-c_2)}{(\beta_{AB} + \xi_{ab})^{1/2}} \right. \\ & \left. - \frac{a(1-c_2)}{(\beta_{AB} + \xi_{ba})^{1/2}} \right\} dx dy dz \quad (5-8) \end{aligned}$$

whereas for the singlet and triplet $1S2P_x$ - BK matrix elements we have

$$\begin{aligned} \frac{H_{BK}}{N} = & A \int_0^1 \int_0^1 \int_0^1 \gamma^2 (1-x)(1-y)(1-z)^2 z^4 \\ & \times \left\{ \frac{bc_1}{(\beta_{AB} + \xi_{ab})^{1/2}} + \frac{ac_1}{(\beta_{AB} + \xi_{ba})^{1/2}} + \frac{b(1-c_2)}{(\beta_{BA} + \xi_{ab})^{1/2}} \right. \\ & \left. + \frac{a(1-c_2)}{(\beta_{BA} + \xi_{ba})^{1/2}} \right\} dx dy dz \quad (5-9) \end{aligned}$$

where the notation in both (5-8) and (5-9) is the same and is defined as follows:

$$a = 2.15, \quad b = 1.19, \quad \alpha_1 = z', \quad \alpha_2 = \frac{1}{2} z'',$$

where the appropriate values of z' and z'' (i.e. whether for singlet or triplet states) are listed in Section 3,

$$C_1 = z(1-xy), \quad C_2 = 1-yz,$$

$$\beta_{AB} = A^2 C_1 (1-C_1) + B^2 C_2 (1-C_2),$$

$$\beta_{BA} = B^2 C_1 (1-C_1) + A^2 C_2 (1-C_2),$$

$$\xi_{ab} = a^2 xyz + \alpha_1^2 yz(1-x) + b^2 z(1-y) + \alpha_2^2 (1-z),$$

$$\xi_{ba} = b^2 xyz + \alpha_1^2 yz(1-x) + a^2 z(1-y) + \alpha_2^2 (1-z),$$

$$N = \frac{29790}{\sqrt{2}} i\pi \quad z' z''^2 (z' z'' ab)^{3/2} \left[\frac{(a+b)^6}{(a+b)^6 + 64(ab)^3} \right]^{1/2} \quad (5-10)$$

Again the evaluation of the corresponding nuclear matrix elements is straightforward but tedious. We note that the symbols ξ_i, F_i, C_1, C_2 and β_m are still defined by eqns. (5-6), (5-3), (5-5), and (5-4) respectively. Also to differentiate between the triplet and singlet contributions we have introduced a symbol

$\tilde{\omega}_i$ defined such that

$$\tilde{\omega}_i = +1 \quad i = 1, 2, 3, 4 \quad \text{for singlet terms}$$

and

$$\begin{aligned} \tilde{\omega}_i &= +1 & i &= 1, 2 \\ &= -1 & i &= 3, 4 \end{aligned} \quad \text{for triplet terms.}$$

Thus for the singlet and triplet $1S2P_z$ states we have

$$H_{(Nuc)} = C B \sum_{i=1}^4 \int_0^1 \int_0^1 \int_0^1 \frac{\tilde{\omega}_i T_i}{F_i^{1/2} \beta_i^9} \left\{ \frac{1}{F_i^2} + \frac{6C_2}{F_i \beta_i^2} + \frac{33C_2^2}{\beta_i^4} \right\} dx dy dz \quad (5-11)$$

where

$$T_1 = T_2 = C_2^3 (1-C_2)(1-x)(1-y)(1-z),$$

$$T_3 = T_4 = C_2^2 y(1-x)(1-y)^2(1-z),$$

while for the singlet and triplet $1S2P_{\chi}$ states the nuclear matrix elements take on the form

$$\begin{aligned} \frac{H_{(NUC)}}{C} = & A \sum_{i=1}^4 \int_0^1 \int_0^1 \int_0^1 \frac{(-1) \tilde{\omega}_i T_i'}{F_i^{1/2} \beta_i^9} \left\{ \frac{1}{F_i^2} + \frac{6C_2}{F_i \beta_i^2} + \frac{33C_2^2}{\beta_i^4} \right\} dx dy dz \\ & - \frac{A}{7} \sum_{i=1}^2 \int_0^1 \int_0^1 \int_0^1 \frac{x^2 y^2 (1-x)^2 (1-y)(1-z)}{\beta_i^7 F_i^{3/2}} \left\{ \frac{5}{F_i^2} + \frac{14C_2}{F_i \beta_i^2} \right. \\ & \left. + \frac{21C_2^2}{\beta_i^4} \right\} dx dy dz \end{aligned} \quad (5-12)$$

where

$$\begin{aligned} T_1' &= T_2' = C_1 C_2^3 (1-x)(1-y)(1-z) \\ T_3' &= T_4' = \gamma C_2 (1-C_1)(1-x)(1-y)^2(1-z) \end{aligned}$$

Now only the numerical integrations on a computer need be done to complete the evaluation of the cross section for capture into the singlet and triplet $1S2P$ states.

-VI- Possible Refinements

The results of the last two chapters were obtained by an application of the first Born approximation. Obviously the use of the second Born approximation, which is equivalent to writing the operator $U(\lambda)$, defined by eqn. (2-5), as

$$U(\lambda) \approx 1 + G_0(\lambda)V, \quad (6-1)$$

would be a formidable task. Hence one is led to search for procedures which are deemed improvements over the first Born approximation but which are still amenable to feasible calculations.

As mentioned in the Introduction the problem of single electron capture by fast protons in hydrogen has been treated by taking into account the distortion produced on the incoming or outgoing waves by the electron-nucleus potential of the bound system. Below we illustrate the matrix elements which would have to be evaluated were this type of refinement to be used in treating two electron capture by fast alpha particles in helium. The system of subscripts used is still that illustrated in Fig. 1. By employing the Chew-Goldberger²¹ identity and following the same procedure of McDowell¹⁰ we may write eqn. (2-8) as

$$\begin{aligned} H_{ba}^+ &= \langle \phi_b' | V' | \bar{\Psi}_a^+ \rangle \\ &= \langle \phi_b' | V_{AB} + V_{A1} + V_{A2} | (\omega_{A1}^+ + \omega_{A2}^+ + \omega_{AB}^+ - 2) \phi_a \rangle \\ &\quad + \text{terms negligible at high energies} \end{aligned} \quad (6-2)$$

where

$$\omega_{ij}^+ = 1 + \frac{V_{ij}}{E - H_0 - V_{ij} + i\epsilon}.$$

Remembering that $\omega_{AB}^+ \rightarrow 1$ at high energies, i.e. there is little distortion of the electron wave function by the internuclear potential, we have

$$H_{ba}^+ = \langle \phi_b' | V_{AB} + V_{A1} + V_{A2} | (\omega_{A1}^+ + \omega_{A2}^+ - 1) \phi_a \rangle. \quad (6-3)$$

In the limit of very high energies $\omega_{A1}^+, \omega_{A2}^+ \rightarrow 1$ and eqn. (6-3) is equivalent to the first Born approximation as we have used it throughout this thesis. It is clear that the computation of H_{ba}^+ from eqn. (6-3) would be a tedious task to say the least.

Another possible refinement might consist of using better variational approximations to the bound states of the helium atom. However in view of the complexity of the results which we have obtained from two-parameter wave functions it is not hard to see that the addition of more parameters to the trial wave functions would increase the complexity of the calculations enormously. In fact one soon reaches the conclusion that due to the many-body aspect of the problem under consideration here any refinement on a first Born approximation calculation might increase the complexity of already arduous computations to perhaps an unjustifiable extent. At any rate the merits of any one refinement will be unclear until the experimental gap is filled in.

-VII- Conclusions and Discussion

It has been seen that the effect of employing an improved atomic wave function for the computation of the cross section for simultaneous capture of two electrons by fast alpha particles in helium does not make a substantial difference over the same cross section computed with the simpler wave function. The small discrepancy between the cross section of GR and our σ_{SIMP} must be interpreted as arising from the various errors inherent in both methods of computation. Thus, for the above type of calculation, it seems unreasonable to bother using a more refined ground state wave function.

Unfortunately the evaluation of matrix elements for capture into the singlet and triplet $1S2P_x$ and $1S2P_z$ states would have been too time consuming with the computational facilities which were available. However since at energies near 0.6 Mev. the cross sections for capture into the triplet $1S2S$ state were found to be about 12% of the ground state value, it would not be unreasonable to expect a contribution of the order of 50% over the energy range from 0.25 to 2 Mev. to the total capture cross section from capture into excited states. It should be recalled that in the energy range 25 - 100 Kev. JS calculated that capture into excited states accounts for one-third of the total cross section for electron capture by protons in atomic hydrogen. It is expected that the numerical calculations for capture into the singlet and triplet $1S2P_x$ and $1S2P_z$ states will be completed in the near future.

One may look forward eventually when reliable experimental cross sections have been measured and the excited states cross sections computations are complete to a settlement of the controversy over when the nucleus-nucleus interaction need not be included in the perturbation Hamiltonian. Certainly the inclusion of this term as in the protons in hydrogen case makes a large difference in the calculated cross section.

Appendix 1

A general method of performing integrations of the type P, Q, R and S listed in Section II is to replace the term $\frac{1}{|\bar{r}_1 - \bar{r}_2|}$ by its equivalent²²

$$\begin{aligned} \frac{1}{|\bar{r}_1 - \bar{r}_2|} &= \frac{1}{r_1} \sum_{l=0}^{\infty} \left(\frac{r_2}{r_1}\right)^l P_l(\cos \theta) \quad , \quad r_1 > r_2 \\ &= \frac{1}{r_2} \sum_{l=0}^{\infty} \left(\frac{r_1}{r_2}\right)^l P_l(\cos \theta) \quad , \quad r_1 < r_2 \end{aligned}$$

where $\cos \theta = \cos(\bar{r}_1, \bar{r}_2)$ and hence

$$\begin{aligned} P_l(\cos \theta) &= P_l(\cos \theta_1) P_l(\cos \theta_2) \\ &+ 2 \sum_{m=1}^l \frac{(l-m)!}{(l+m)!} P_l^m(\cos \theta_1) P_l^m(\cos \theta_2) \cos m(\varphi_1 - \varphi_2) . \end{aligned}$$

It is clear that if in integrals of the form

$$I = \int \frac{F_1(\bar{r}_1) F_2(\bar{r}_2)}{|\bar{r}_1 - \bar{r}_2|} d\bar{r}_1 d\bar{r}_2$$

either F_1 or F_2 (or both) are spherically symmetric functions only the $l=0$ terms will contribute to the integral and hence the integrations become trivial.

The integral P can be essentially resolved into three parts denoted

$$\begin{aligned} K_0 &= \int \frac{1}{|\bar{r}_1 - \bar{r}_2|} e^{-(\alpha_1 r_1 + \alpha_2 r_2)} d\bar{r}_1 d\bar{r}_2 \quad , \\ K_1 &= \int \frac{r_2}{|\bar{r}_1 - \bar{r}_2|} e^{-(\alpha_1 r_1 + \alpha_2 r_2)} d\bar{r}_1 d\bar{r}_2 \quad , \\ K_2 &= \int \frac{r_2^2}{|\bar{r}_1 - \bar{r}_2|} e^{-(\alpha_1 r_1 + \alpha_2 r_2)} d\bar{r}_1 d\bar{r}_2 \quad . \end{aligned}$$

Using the above method K_0 is easily evaluated as

$$K_0 = 32\pi^2 \frac{(\alpha_1^2 + 3\alpha_1\alpha_2 + \alpha_2^2)}{(\alpha_1\alpha_2)^2(\alpha_1 + \alpha_2)^3}$$

whence

$$K_n = (-1)^n \frac{\partial^n}{\partial \alpha_z^n} (K_0)$$

Integrals occurring in the evaluation of Q are of the form

$$Q_{mn} = \int \frac{r_1^m r_2^n}{|\vec{r}_1 - \vec{r}_2|} e^{-\alpha(r_1+r_2)} d\vec{r}_1 d\vec{r}_2, \quad m, n = 0, 1, 2, \dots$$

These are readily evaluated by considering

$$Q'_{mn} = \int \frac{r_1^m r_2^n}{|\vec{r}_1 - \vec{r}_2|} e^{-(\alpha_1 r_1 + \alpha_2 r_2)} d\vec{r}_1 d\vec{r}_2, \quad m, n = 0, 1, 2, \dots$$

whence $Q'_{00} = K_0$ is used to yield the result

$$Q_{mn} = (-1)^{m+n} \frac{\partial^{m+n}}{\partial \alpha_1^m \partial \alpha_2^n} Q'_{00} \Big|_{\alpha_1 = \alpha_2 = \alpha}$$

The validity of this procedure is easily checked by evaluating a few of the

Q_{mn} 's by an alternate method, i.e. by expressing the terms occurring in

the integrand by their respective Fourier transforms and then integrating the resultant expression.

The integral R, apart from a factor introduced by the $\cos^2 \theta_2$ term is identical in form to K_2 . In S however only the $l=1$ term in the expansion of $\frac{1}{|\vec{r}_1 - \vec{r}_2|}$ will contribute and the integral

$$S_{11} = \int \frac{r_1 r_2}{|\vec{r}_1 - \vec{r}_2|} e^{-\alpha(r_1+r_2)} \cos \theta_1 \cos \theta_2 d\vec{r}_1 d\vec{r}_2$$

is readily evaluated yielding

$$S_{11} = \frac{28 \pi^2}{3 \alpha^7}$$

Appendix 2

The following three dimensional Fourier transforms were found useful in reducing the BK and nuclear matrix elements:

$f(\vec{r})$	$g(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int f(\vec{r}) e^{-i\vec{k}\cdot\vec{r}} d\vec{r}$
$\frac{e^{-\beta r}}{r}$	$\left(\frac{2}{\pi}\right)^{1/2} \cdot \frac{1}{(\beta^2 + k^2)}$
$\frac{1}{r}$	$\left(\frac{2}{\pi}\right)^{1/2} \cdot \frac{1}{k^2}$
$e^{-\beta r}$	$\left(\frac{2}{\pi}\right)^{1/2} \cdot \frac{2\beta}{(\beta^2 + k^2)^2}$
$r e^{-\beta r}$	$\left(\frac{2}{\pi}\right)^{1/2} \left[\frac{8\beta^2}{(\beta^2 + k^2)^3} - \frac{1}{(\beta^2 + k^2)^2} \right]$
$r^2 e^{-\beta r}$	$\left(\frac{2}{\pi}\right)^{1/2} \left[\frac{48\beta^3}{(\beta^2 + k^2)^4} - \frac{24\beta}{(\beta^2 + k^2)^3} \right]$
$z e^{-\beta r}$	$\left(\frac{2}{\pi}\right)^{1/2} \cdot \frac{8i\beta k_z}{(\beta^2 + k^2)^3}$
$xz e^{-\beta r}$	$-\left(\frac{2}{\pi}\right)^{1/2} \cdot \frac{48\beta k_x k_z}{(\beta^2 + k^2)^4}$
$z^2 e^{-\beta r}$	$\left(\frac{2}{\pi}\right)^{1/2} \left[\frac{8\beta}{(\beta^2 + k^2)^3} - \frac{48\beta k_z^2}{(\beta^2 + k^2)^4} \right]$

Appendix 3

All forms of the Feynman auxiliary integral may be obtained from the simple identity

$$\frac{1}{ab} = \int_0^1 \frac{dx}{[ax + b(1-x)]^2} \quad .$$

Repeated differentiation with respect to a and b gives the general form

$$\frac{1}{a^m b^n} = \frac{(m+n-1)!}{(m-1)!(n-1)!} \int_0^1 \frac{x^{m-1} (1-x)^{n-1} dx}{[ax + b(1-x)]^{m+n}} \quad .$$

By writing

$$\frac{1}{abc} = \int_0^1 \frac{dx}{[ax + b(1-x)]^2 c} = \int_0^1 \frac{dx}{q^2 c}$$

and then using the integral representation for $1/q^2 c$ we get

$$\frac{1}{abc} = 2 \int_0^1 \int_0^1 \frac{y dx dy}{[axy + by(1-x) + c(1-y)]^3} \quad .$$

Again repeated differentiation yields

$$\frac{1}{a^m b^n c^k} = \frac{(m+n+k-1)!}{(m-1)!(n-1)!(k-1)!} \int_0^1 \int_0^1 \frac{x^{m-1} y^{m+n-1} (1-x)^{n-1} (1-y)^{k-1} dx dy}{[axy + by(1-x) + c(1-y)]^{m+n+k}} \quad .$$

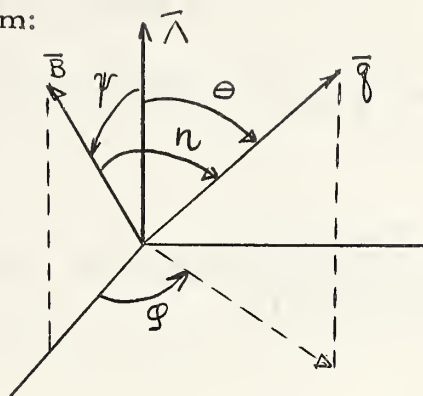
Similarly one obtains the useful representation

$$\frac{1}{a^m b^n c^k d^l} = \frac{(m+n+k+l-1)!}{(m-1)!(n-1)!(k-1)!(l-1)!}$$

$$\times \int_0^1 \int_0^1 \int_0^1 \frac{x^{m-1} y^{m+n-1} z^{m+n+k-1} (1-x)^{n-1} (1-y)^{k-1} (1-z)^{l-1} dx dy dz}{[axyz + byz(1-x) + cz(1-y) + d(1-z)]^{m+n+k+l}} \quad .$$

Appendix 4

The integral $J_l^{(z)}$ defined by eqn. (5-7) is readily evaluated by employing the following coordinate system:



since

$$q_z = q \cos \eta = q [\cos \psi \cos \theta + \sin \psi \sin \theta \sin \phi]$$

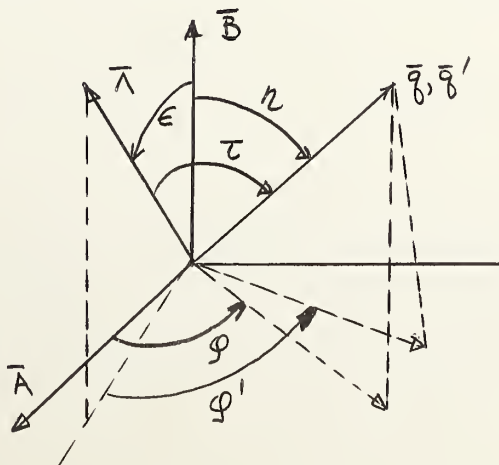
the integration over the azimuthal angle ϕ will vanish and we are left with

$$\begin{aligned} J_l^{(z)} &= \cos(\bar{B}, \bar{\lambda}) \int \frac{q \cos \theta d\bar{q}}{[(\bar{q} + \bar{\lambda})^2 + \gamma^2]^{\frac{1}{2}}} \\ &= -\pi^2 c_2 B \frac{(2l-5)!!}{(l-1)! 2^{l-2} \gamma^{2l-3}} \end{aligned}$$

With the aid of the coordinate system below in which $\bar{\lambda}$ lies in the $\phi = 0$ plane and ϕ' is the azimuthal angle of \bar{q}' in the plane perpendicular to

$\bar{\lambda}$ we may express q_y as

$$q_y = q \sin \eta \sin \phi = q' \sin \tau \sin \phi'$$



Hence due to the integration over φ' the integral $J_\ell^{(y)}$ is zero. The projection g_x may be written as

$$\begin{aligned} g_x &= g \sin \tau \cos \varphi \\ &= g' [\cos(\bar{\lambda}, \bar{B}) \sin \tau \cos \varphi' + \sin(\bar{\lambda}, \bar{B}) \cos \tau] . \end{aligned}$$

Thus

$$\begin{aligned} J_\ell^{(x)} &= \sin(\bar{\lambda}, \bar{B}) \int \frac{g' \cos \tau \, d\varphi'}{[(\bar{q}' + \bar{\lambda})^2 + \gamma^2]^\ell} \\ &= -\pi^2 C_1 A \frac{(2\ell-5)!!}{(\ell-1)! 2^{\ell-2} \gamma^{2\ell-3}} . \end{aligned}$$

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